

Phase Distribution in a Disordered Chain and the Emergence of a Two-parameter Scaling in the Quasi-ballistic to the Mildly Localized Regime

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Abstract

We study the phase distribution of the complex reflection coefficient in different configurations as a disordered 1D system evolves in length, and its effect on the distribution of the 4-probe resistance R_4 . The stationary ($L \rightarrow \infty$) phase distribution is almost always strongly non-uniform and is in general double-peaked with their separation decaying algebraically with growing disorder strength to finally give rise to a single narrow peak at infinitely strong disorder. Further in the length regime where the phase distribution still evolves with length (i.e., in the *quasi-ballistic* to the *mildly localized* regime), the phase distribution affects the distribution of the resistance in such a way as to make the mean and the variance of $\log(1 + R_4)$ diverge independently with length with different exponents. As $L \rightarrow \infty$, these two exponents become identical (unity). Obviously, these facts imply two relevant parameters for scaling in the quasi-ballistic to the mildly localized regime finally crossing over to one-parameter scaling in the strongly localized regime.

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Evolution of the reflectance (or, the two-probe resistance, R) and the phase (ϕ) of the complex reflection coefficient [$r = R^{1/2} \exp(i\phi)$] with length (L) due to backscattering in a disordered quantum conductor are intimately connected. Indeed one is coupled to the other as demonstrated clearly, e.g., in the coupled differential equations for these quantities obtained by using the invariant imbedding method [1, 2, 3]. It may be noted here that for a single disordered sample, as opposed to an ensemble of them, there is no finite phase decoherence length at zero temperature. Since phase coherence is of paramount importance in disordered systems, the important object to look for is the distribution of the phases in different configurations and its evolution with length (L). It is thus intriguing to note that even though a lot of work has been done for the last three to four decades on the resistance and its moments (and on its probability density as well), comparatively little has been done on the phase distribution and its evolution with length (L). While rigorous results exist for exponential localization in 1D, i.e.,

$$R(L) \sim \exp(2\alpha L), \quad (1)$$

in the $L \rightarrow \infty$ limit ($\xi = 1/\alpha$ being the localization length), and field-theoretic and numerical methods indicate an insulator to metal transition only above 2D (at least in the absence of any magnetic or other fields which break the time-reversal invariance and of spin-orbit scattering [4]), no analytic or otherwise fully definitive result for the phase distribution covering the complete domain of real space or disorder strength exists even in 1D. Notwithstanding this fact, almost all analytic works assume random [5] (uniform) distribution of the phase angle between 0 and 2π to solve for the distribution of the resistance. It is sometimes called the random phase model. In the first half of this Letter, we first concentrate on the evolution of the phase distribution (in a disordered 1D system) with L and study how the peaks in the stationary ($L \rightarrow \infty$) phase distribution behave as the disorder strengths are varied from weak to infinitely strong. Since the phase distribution for a very large length keeps changing with disorder strength, clearly a large length scale should

not necessarily imply a large disorder scale even in 1D. In the latter half of this work, we come back to moderate length scales where the phase distribution is still evolving with length and study its effect on the first two moments of the logarithmic resistance. The main result of this work is that in this regime, the above two moments diverge with different exponents contrary to the case of a *log-normal* distribution where there should have been a single exponent. Also, interestingly, for very large length scales ($L \gg \xi$), the above two moments diverge with the same exponent (as in the case of a *log-normal* distribution) even though the stationary phase distribution is far from uniform. Hence our conclusion below that as long as the non-uniform phase distribution does not settle down to its stationary limit, the logarithmic resistance distribution gets affected in such a way that its description requires at least two independent scaling parameters and not one.

The first definitive work on the issue of the phase distribution seems to be the numerical transfer matrix work of Stone, Allan and Joannopoulos [6] (referred to as SAJ from now on) which indicates very clearly that this distribution [7] is far from uniform except in the *diffusive* (disordered metallic) regime. As a matter of fact, it was shown by SAJ that for disorder or length scale much smaller than that for the diffusive regime (i.e., *quasi-ballistic* in the current terminology), the phase angle distribution is doubly peaked around $\phi = \frac{\pi}{2}$ and $\phi = \frac{3\pi}{2}$ respectively. We note that very recently this result was obtained analytically by Heinrichs [8] by solving the invariant imbedding equations exactly in the limit $L \ll (2k_F)^{-1} < \xi$, where k_F is the Fermi wave-vector of the incoming electrons from a semi-infinite perfect lead attached to the source reservoir of the electrons. It is only in the regime $(2k_F)^{-1} \ll L < \xi$ that the system is diffusive (or, quasi-metallic) and the phase distribution is nearly uniform. This is the so-called *weak localization regime*. In 1D, the two-probe conductance (transmittance) in this regime also follows a nearly uniform distribution [9] and thus gives rise to a universal conductance fluctuation (UCF) appropriate for 1D [10]. But what happens to the phase for $L \gg \xi$ and $W \rightarrow \infty$ seems to be somewhat controversial (here W is the strength of the disorder

as measured by the width of the randomness characterizing the problem). This is important because, as we discussed before, two very different distributions in ϕ should affect the stationary ($L \rightarrow \infty$) distribution of R differently and the effect should be clearly seen in the ensemble-averaged value of the resistance. The old SAJ result indicates that the stationary phase distribution in the strong localization (very large disorder) limit becomes sharply peaked (single peak) at an angle dependent only on the Fermi energy of the electron but independent of W . But, there also exists an opposite view [11] that in the strong disorder limit the stationary distribution becomes doubly peaked.

In the first part of this Letter we investigate this controversial issue in the very large length scale or the fully localized regime (in 1D). We work within a single band tight binding hamiltonian on a lattice with a lattice constant $a = 1$ to set the length scale, the nearest neighbour hopping term $V = 1$ to set the energy scale, and an uniform random distribution in the site energy: $P(\epsilon_n) = \frac{1}{W}$, in the domain $[-\frac{W}{2}, \frac{W}{2}]$, and zero elsewhere. Thus $\frac{W}{V}$ serves as a measure of the strength of disorder. A transfer matrix method described elsewhere [10] has been used to solve for the complex reflection coefficient r of the sample attached to semi-infinite perfect leads. The phase ϕ is calculated from the real and imaginary parts of r and properly shifted into the domain $[0, 2\pi]$. For our calculation of phases, we have worked with 5,000 – 25,000 configurations (larger the disordered chain length, larger the number), and chose lengths such that the distribution does not change significantly on increasing the length further. Thus the histograms we present below do indeed refer to the stationary distributions of the phase, $P(\phi)$, in the medium to very strong localization regime. Further, all the histograms have been normalized for the purposes of comparison.

In Fig.1 we show the stationary distribution of phase at the Fermi energy $E_F = 1.6V$ for different disorders ranging from $\frac{W}{V} = 3$ to $\frac{W}{V} = 200$. The localization length is found to vary from $\xi \simeq 3a$ to $\xi \simeq 0.12a$ in this range. There are several features to be noticed from these histograms. The phase distribution is already very

non-uniform for $\frac{W}{V} = 3$, and it has two broad peaks one about twice in altitude than the other. As the disorder grows to $\frac{W}{V} = 8$ (Fig. 1b), the non-uniformity in $P(\phi)$ becomes more pronounced. The peaks become narrower and stronger (at the cost of a reduction in the background). Individually the weaker peak grows more in strength, and thus the strength of the two peaks tend to approach each other. Most importantly, they come closer as W increases. This trend continues upto $\frac{W}{V} = 60$ (Fig. 1e), where one can still distinguish between these two peaks very close in strength and position in the phase domain. Finally for $\frac{W}{V} = 200$ (Fig. 1f), we cannot distinguish between the two peaks for our chosen bin size of $\frac{\Delta\phi}{2\pi} = 0.01$, and the distribution becomes a very strongly peaked function. For our accuracy, this disorder seems to be *infinitely* strong. We did also look at the position of this single peak for infinitely strong disorder, and find that it appears at $\phi_\infty = 2\cos^{-1}\frac{E_F}{2}$. For example, the peak in Fig. 1f appears at $\phi_\infty = 1.29$ radian. This result may be analytically calculated exactly from the fact that for an infinitely strong disorder ($W \rightarrow \infty$), the electron gets almost completely backscattered from a single (the first in the chain) impurity itself. One may thus look at a single, infinitely strong disorder in the middle of an otherwise ordered chain, and obtain the above result exactly. Interestingly ϕ_∞ lies in between the two peaks for any particular disorder in Figs. 1a-1e. It may be noted here that the appearance of the two peaks for large lengths and for intermediate disorder was previously reported in the literature [12] as a passing remark. In that work, done only at one E_F , the second peak was just a very mild hump, whose strength was reported to be decreasing (finally vanishingly small) with disorder and hence all the emphasis was given to the single strong peak and the variation of its position with W . In contrast, we find that at any fixed E_F , the strength of the weaker peak grows stronger and the two peaks move (as if attracted) towards each other with increasing W (see Fig. 1), and finally the two peaks coalesce to give a single peak for infinitely strong disorders.

Obviously the next question would be how does the two peaks in the stationary distribution approach each other as W increases. For this purpose, we have studied

the histograms as in Fig.1 at other energies and find that as one approaches closer to the band center (i.e., $|E_F| \rightarrow 0$), the onset disorder for the appearance of two peaks (in the medium strong disorder regime) becomes larger. For example for $\frac{E_F}{V} = 1.6$, this onset value is $\frac{W}{V} \simeq 3$ but for $\frac{E_F}{V} = 0.1$, the onset value is $\frac{W}{V} \simeq 5$. Further whereas the peaks have unequal strengths when the Fermi energy is away from the band center, on approaching the band center the two peaks assume near identical strengths even near the onset disorder. Thus except for the ‘mass’ center (ϕ_∞) and the relative ‘masses’ of the two peaks, the sequence of histograms at any energy look quite similar to those in Fig. 1. For the purposes of illustration we have chosen both the energies mentioned above. In Fig. 2a, we have plotted the relative positions of the left and the right peaks with respect to ϕ_∞ (to look for asymmetry in their positions) as a function of $\frac{W}{V}$ at the energy $\frac{E_F}{V} = 0.1$ and in Fig. 2b we have done the same for $\frac{E_F}{V} = 1.6$. The excellent linear fits for both the sets and their near-parallelity on the log-log plot clearly indicate a power law with the same exponent. The results may be summarized as follows. For $L \gg \xi$, we find that the asymptotically stationary phase distribution is in general a two-peaked function with the left and the right peaks at

$$\phi_{r,l} = \phi_\infty \pm \frac{b_{r,l}}{W^\mu}, \quad (2)$$

where b_l and b_r are constants independent of $\frac{W}{V}$ but dependent only on $\frac{E_F}{V}$, whereas μ is a constant independent of $\frac{W}{V}$ or $\frac{E_F}{V}$ (+ for r and $-$ for l -peaks). For the case in Fig. 2a where $\frac{E_F}{V} = 0.1$, we have $b_l \simeq b_r = 0.50$, and $\mu = 0.85$. For Fig. 2b where $\frac{E_F}{V} = 1.6$, we still have $\mu = 0.85$, but $b_l = 0.37$ and $b_r = 0.28$. Very similar results are obtained at any other energy. The inequality of b_l and b_r away from the band center indicate that the peaks are asymmetrically separated from their fixed asymptotic ($W \rightarrow \infty$) position. This asymmetry seems to be correlated to the inequality in peak-strengths at finite strengths at finite W ’s and for energies away from the band center. It may be noted that the eq.(2) indicates that as W increases, the separation between the peaks decays as:

$$\Delta\phi = \frac{b}{W^\mu}, \quad (3)$$

where $b = b_l + b_r$. Let us now look at a simple consequence. The renormalization group flow in the one-parameter scaling [13] in 1D would have us believe that increasing the length scale is equivalent to increasing the disorder scale. But Eq.(2) implies that different disorder strengths give rise to different stationary ($L \rightarrow \infty$) phase distributions and hence indicates that, contrary to the one-parameter scaling, a large length scale is not completely equivalent to a large disorder scale.

To be more sure of the effects of the still-evolving strongly non-uniform phase distribution, we study in this latter half of our work, the evolution of the logarithmic resistance in the domain where stationarity is not yet reached. In particular we are interested in testing the validity or the lack thereof of the one-parameter scaling theory [13]. Let us explain our motivation clearly. It is well-known that resistance (or, conductance) of a disordered system is not self-averaging in the sense that its distribution has a log-normal tail even in the metallic regime, and becomes completely log-normal in the localized regime [14]. Here the word log-normal means that the random variable $u(L) = \ln(1 + R_4) = -\ln T(L)$, where $R_4(L) = R(L)/T(L)$ is the four-probe resistance and $T(L) = 1 - R(L)$ is the two-probe conductance, has a normal distribution. Now in most of the previous analytical works [5], a uniform random distribution for ϕ is assumed, and one then obtains the result that the two parameters of $P_L(u)$, namely the mean and the variance diverge linearly with L . As in any normal distribution, they diverge with the same exponent (i.e., exactly unity), and hence one obtains only one relevant parameter in the scaling of the resistance. The main result of this Letter as shown below is that in the *regime where $P_L(\phi)$ is both non-uniform and is changing with L* , the mean and the variance of u diverge with different exponents and hence in that regime *the one-parameter scaling does not seem to hold*. Of course this state of affairs does not hold for $L \gg \xi$, and we show that in this regime where $P_L(\phi)$ is independent of length, i.e., *stationary* (although far from uniform), the mean and the variance of $u(L)$ do again diverge as

L consistent with one-parameter scaling in the very large length scale or very strong disorder regime.

For our purpose we calculate $R_4(L)$ for 20,000-40,000 configurations as a function of L at the Fermi energy $\frac{E_F}{V} = 1.6$ and a disorder strength $\frac{W}{V} = 1$. Then we calculate the mean $\langle u \rangle$ and the variance $var(u) = \langle u^2 \rangle - \langle u \rangle^2$ as a function of L . It may be pointed out that in this case $P_L(\phi)$ does not assume its stationary form, i.e., $P(\phi)$, until a length of about $L = 300$. From the exponential drop of the average reflectance we find that the localization length is $\xi \simeq 40$ and the $P_L(\phi)$ is double peaked (figure not shown here for brevity) even in the quasi-ballistic as well as the weakly localized regime. As a result the probability density of the logarithmic resistance, $P_L(u)$, is strongly asymmetric in the entire range of length ($L = 10 - 700$) studied even though the asymmetry gradually becomes smaller with increasing L . Thus in contrast to all the previous works known to the author, $P_L(u)$ is non-Gaussian even in the weakly localized regime. More details on this will be discussed elsewhere. For the purpose of this Letter, we show in Fig.3 the log-log plot for the $\langle u \rangle$ and the $var(u)$ as a function of L . We find that whereas $\langle u(L) \rangle = 0.058L$ indicating pure exponential growth in the entire domain, $var(u)$ first goes as $0.0075L^{1.57}$ upto $L \simeq 80$ (2ξ) and crosses over towards $0.11L$ for $L \geq 300$. It is interesting to note that the graphs for $\langle u \rangle$ and $var(u)$ cross each other at $L = \xi \simeq 40$. Thus $\langle u \rangle$ and $var(u)$ diverge with two independent exponents, namely 1 and 1.57 respectively, from the quasi-ballistic through the quasi-diffusive to the mildly localized regime (upto about 2ξ). In this regime, the first two moments of $P_L(u)$, i.e., $\langle u \rangle$ and $var(u)$, behave as two independent parameters (as opposed to a gaussian behaviour) or relevant variables for scaling and hence the one-parameter scaling does not seem to adequately describe the transport properties. Whether these two are the only relevant variables in this regime is related to the nature of the deviation of $P_L(u)$ from gaussianity and needs to be studied more carefully. Also it may be noted (Fig. 3) that for $L \geq 7\xi$, the phase distribution $P(\phi)$ is stationary, and both $\langle u \rangle$ and $var(u)$ diverge identically (i.e., linearly) indicating

that there is just one relevant variable (e.g., only the $\langle u \rangle$), and the one-parameter scaling theory is valid for very large length scales. In this connection it may be noted that in one of our previous works [15] on conductance and its fluctuations from the quasi-ballistic to the diffusive regime, we did find the existence of two independent length scales, namely ξ and a quasi-ballistic length scale $\Delta(W)$ which is essentially a periodicity length of conductance oscillations. It is interesting to note that the effect of this extra length scale Δ may also be discerned only upto $L \simeq \xi$, since the conductance oscillations become imperceptible beyond that length. The two independent parameters in the form of length scales should show up in conductance measurements. The measurements could be quite tricky though since the amplitude of oscillation depends upon how much the hopping term (or, the effective electronic mass) in the sample differs from that in the connecting leads. If this difference is not large enough, the UCF may mask the oscillations, i.e., the other length scale completely [15].

We stress again that our aim was not to find the inadequacy of the one-parameter scaling in the thermodynamic limit, but rather to find why and where could this breakdown occur. Our findings suggest that this occurs for moderate disorders and near the onset of the metal-insulator transition where the phase distribution still evolves with length. It is true that a quantum phase transition from an insulator to a metal does not take place in 1D in the thermodynamic limit, and hence the effect mentioned above looks like a crossover effect. But it is also true that on renormalization from a small to a large length scale, the 1D system flows from the weakly localized to the strongly localized regime qualitatively similarly to that for a 2D or for a $(2 + \epsilon)$ -dimensional system on the localized side of the mobility edge E_c (but initially very close to it). On qualitative grounds, we believe that the phase distribution will evolve in the latter two cases just as in 1D. Thus we expect a two-parameter scaling similar to the one discussed above in 2D as well as in $(2 + \epsilon)$ dimension on the localized side. The non-trivial second exponent (of $\text{var}(u)$) would be Fermi-energy-dependent as in above. Further we conjecture that on the extended

side of E_c but close to it, $\langle u \rangle$ and $\text{var}(u)$ would diverge independently and one would find two independent exponents in the distribution. But on renormalization, one would again scale far away from E_c on the extended side (since one is not sitting exactly on the E_c), the behavior would again *crossover* to a qualitatively different one, namely that $\langle u \rangle$ would diverge logarithmically and $\text{var}(u)$ would tend to vanish (consistent with an Ohmic behavior, which is our guiding principle in this asymptotic limit). Further work needs to be done in this area.

As a further support, we indicate a possible relation of our results to a recent novel work [16] on 3D disordered systems, where it has been shown using supersymmetric non-linear sigma model, that the *level spacing distribution close to E_c is quite non-standard* in the sense that the distribution is non-Wigner-Dyson in the disordered metallic side and non-Poissonian in the insulating side. The first thing to note is that this behavior would also look like a crossover phenomenon in the length scale (as discussed above) since on renormalization one goes far away from E_c and the non-standard behavior would predictably crossover to one of the standard forms (Wigner-Dyson or Poisson). Second, if one notes that the electronic conduction (say, using Kubo formula) would require the hopping of the electron between two energy levels on either side of the Fermi energy, it becomes clear that this process really samples the level spacing distribution around E_F . Thus if E_F is close to E_c and if something unusual is happening in the level spacing distribution around the latter, the distribution and the scaling properties of the conductance should also become unusual there (e.g., neither Ohmic nor log-normal as in our case), and *vice-versa*. The relation between the level spacing distribution and the conductance distribution would be explored further in the future.

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Figure Captions:

Fig. 1 Normalized histograms representing the stationary ($L \rightarrow \infty$) phase distributions at $E_F/V = 1.6$ and at an increasing sequence of disorder in (a) to (f).

Fig. 2 Double logarithmic plots of the relative positions of the left and the right peaks ($|\phi_{l,r} - \phi_\infty|$) in the stationary ($L \rightarrow \infty$) phase distribution as a function of the disorder strength W/V at two different energies: (a) for $E_F/V = 0.1$, the peaks are nearly symmetrically placed, and (b) for $E_F/V = 1.6$, the peaks are asymmetrically placed about ϕ_∞ .

Fig. 3 Double logarithmic plots of the mean and the variance of the logarithmic four-probe resistance, $u = \log(1 + R_4)$ as a function of length L for $E_F/V = 1.6$. While $\langle u \rangle$ diverges as L all the way from the quasi-ballistic to the strongly localized regime, $\text{var}(u)$ diverges with an exponent of 1.57 in the regime from the quasi-ballistic to the mildly localized ($L \simeq 2\xi$) and then crosses over to a divergence as L in the strongly localized regime.